LQCD-ext II Project
2015 Annual Review

Overview and USQCD Management

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For USQCD
http://www.usqcd.org

LQCD-ext II Project 2015 Annual Review
Brookhaven
May 21-22, 2015

Synopsis

- First annual review of the LQCD-ext II lattice computing hardware project, 2015-19.
  - Hardware is located at BNL, JLab, Fermilab.
  - Projects funded jointly by DoE's offices of HEP and NP.
    - LQCD-ext II, total budget $14.0 M - under review today.
    - Follow-on to the LQCD and LQCD-ext Projects.
- The LQCD Project is one of several hardware and software efforts overseen by USQCD.
- USQCD is an umbrella group consisting of most US lattice gauge theorists. Its purpose is to develop the software and hardware infrastructure required for lattice gauge theory calculations.

Plan of talks

(Detailed schedule at http://projects.fnal.gov/lqcd/reviews/May2015Review/agenda.shtml .)

May 21

08:30	Welcome (15 min) – *Robert Tribble, Deputy Director for Science and Technology, BNL*
08:45	Executive session (45 min)
09:30	Logistics and Introductions (5 min) – *Bill Boroski*
09:35	LQCD-ext II Overview, USQCD Governance (incl. Allocations) (55 min) – *Paul Mackenzie*
10:30	Break (15 min)
10:45	Science Talk 1: Cold Nuclear Physics (30 min) – *Will Detmold*
11:15	Science Talk 2: QCD Thermodynamics (30 min) – *Frithjof Karsch*
11:45	Science Talk 3: Beyond the Standard Model (20 min) – *Anna Hasenfratz*
12:05	Lunch / Executive Session
1:05	Science Talk 4: QCD for Particle Physics (40 min) – *Andreas Kronfeld*
1:45	LQCD-Ext: Technical Performance of FY14 Cluster Deployment (15 min) – *Amitoj Singh*
2:00	LQCD-Ext: Project Close-out (30 min) – *Bill Boroski*
2:30	Coffee Break (15 min)
3:20	LQCD-Ext II: Project Management and Performance (60 min) – *Bill Boroski / Rob Kennedy*
3:40	LQCD-Ext II: FY16 Hardware Acquisition Planning (30 min) – *Chip Watson*
4:15	Executive Session (60 min)
5:15	Committee request for additional information – *Review Committee & Project Leadership*
6:00	Adjourn
7:00	Dinner

Overview

Scientific achievements

LQCD Project management and technology

USQCD

- Organizes computing hardware and software infrastructure for lattice gauge theory in the US.
- Represents almost all of the lattice gauge theorists in the US; ~ 160 people.
    - ~ 100 participating in physics proposals in a typical year.
- Physics calculations are done by smaller component collaborations within USQCD:
    - Fermilab, HotQCD, HPQCD, HadSpec, LHPC, LSD, MILC, NPLQCD, RBC, ...
    - These are the core entities of the US lattice community.

USQCD timeline

- USQCD formed in 1999.
- LQCD, LQCD-ext, and LQCD-ext II Projects capacity hardware grants from HEP and NP.
  - Being reviewed today.
  - Installed at JLab, Fermilab, and BNL.
- INCITE grants since 2008.
  - For our largest-scale jobs; jobs that can’t be done on smaller computers.
- SciDAC software grants since 2001.
  - Essential for making effective use of Leadership Computing Facilities and our dedicated hardware, and for accomplishing our physics objectives.

Achievements 2005-2015

- In HEP, lattice-QCD calculations played a critical role in making the flavor-physics program of the B factories and the Tevatron a success.
- In NP, lattice QCD played a key role in motivating the experimental physics programs of RHIC and the 12-GeV upgrade, and it solidly nailed down the QCD deconfinement temperature, a key quantity in interpreting the results of heavy-ion collisions at RHIC.

Opportunities, 2015-2019

- In 2015, our opportunities are broader and deeper than ever before.
- In nuclear physics,
  - Solid calculations of the hadronic resonance spectrum are needed to guide the search for hybrid states in the resonance region.
  - Calculations of the equation of state at non-zero baryon density and cumulants of conserved charge fluctuations are needed to guide the exploration of the QCD phase diagram with the heavy ion program at RHIC.
  - We are now in a position to envision the calculation of the spectra and structure of nuclei from first principles, with lattice QCD at its foundation. It will take years to make this a reality.
- In particle physics, lattice QCD calculations are needed in applications large and small throughout the coming experimental program, like perturbative QCD.

USQCD

LQCD-ext II Project

LQCD Federal project director: John Kogut (HEP)
LQCD Federal project monitor: Elizabeth Bartosz (NP)

USQCD Executive Committee: Paul Mackenzie (chair), Rich Brower, Norman Christ, Frithjof Karsch, Julius Kuti, Kostas Orginos, David Richards, Martin Savage, Bob Sugar

LQCD Contract project manager: Bill Boroski
LQCD Associate project manager: Rob Kennedy

USQCD Software Committee: Rich Brower (chair)

USQCD Scientific Program Committee: Anna Hasenfratz (chair)

Green: USQCD present today.

USQCD is funded through SciDAC, through the LQCD project, and through base HEP and NP funds at BNL, Fermilab, and JLab.

USQCD web page: http://www.usqcd.org.

Organization, goals, allocations the Charter of USQCD

http://www.usqcd.org/documents/charter.pdf

Charter of USQCD

December, 2014

USQCD

USQCD is a consortium of all the collaborations and nearly all the individuals in the US using lattice field theory techniques to solve fundamental problems in high energy and nuclear physics. USQCD organizes the hardware and software infrastructure needed by the United States lattice gauge theory community for the study of Quantum Chromodynamics (QCD), the theory of the strong interactions of subatomic physics, and other theories that have been proposed to explain physics beyond the standard model. The USQCD Executive Committee was formed to provide leadership in developing this computational infrastructure. USQCD receives primary funding from the DOE's LQCD computing hardware Project and SciDAC software program, as well as computing time from the DOE INCITE Program and from the NSF. In accordance with USQCD's original mandate, these resources are available to all members of the US lattice community. Membership in USQCD is open to all US lattice gauge theorists, and almost all US lattice gauge theorists are members. USQCD organizes this infrastructure nationally and sets the broad physics goals of the US lattice program. These goals are chosen to address outstanding research opportunities presented by the national and international programs in high energy and nuclear physics and to represent the goals and capabilities of the physics collaborations and individuals who make up USQCD. The actual research using the USQCD hardware and software infrastructure is carried out and published by these collaborations and individuals within USQCD.

This document describes the current procedures of USQCD. These procedures have evolved over the life of USQCD in response to suggestions of review panels at the Annual Progress Reviews of the LQCD computing hardware IT Project, and as a results of discussions with USQCD members at All Hands meetings. We expect them to continue to gradually evolve in the future.

The Executive Committee

The Executive Committee of USQCD provides leadership for and manages USQCD. The

This year, we have written down many of the USQCD practices and procedures that have been discussed informally with USQCD members and with previous review committees, and placed them publicly online.

Organization

- In 2003 when USQCD hardware funding began, Peter Rosen (head of HEP and NP) made it clear that DoE expected the hardware to be operated as a national facility.
  - Open to all in US to submit proposals.
  - USQCD is like Fermilab fixed-target facilities, not like CMS or GlueX.
  - Overall physics goals are set by USQCD in our white papers and proposals for hardware and software, but specific projects are developed by component collaborations like MILC, RBC, NPLQCD, HOTQCD, ..., or by individuals and allocated by SPC. (Role of EC in this process is analogous to that of lab director.)

- This model has worked very well.
  - Young people can be PIs of their own physics programs as soon as they are able to formulate a project and a proposal that is convincing to the Scientific Program Committee.
    - They can be recognized for their own scientific programs much more easily than as part of a hundred-member collaboration.
    - The five people who got junior faculty or staff jobs in the last couple years all served as PIs of their own proposals; two of them with no senior collaborators.
  - When groups disagree on methods, they can compete.
  - We have been very productive under this model.

Executive Committee

Paul Mackenzie (chair), Rich Brower, Norman Christ, Frithjof Karsch, Julius Kuti, Kostas Orginos, David Richards, Martin Savage, Bob Sugar

Present today.

- Provides overall leadership for USQCD and point of contact for the DoE.
- Organizes the writing of the proposals for hardware and software and of the white papers and chooses the members of the other committees.

Executive Committee

- Rotates new members at ~ one/year.
  - Close to full rotation over ~ 10 years is planned. Over half have rotated already.
  - The EC rotates in a way that preserves rough balance. Current practice: approximate balance between HEP and NP, one member from each of the half dozen largest physics collaborations, one member from each of the three partner labs, a few members from outside these groups.
  - This year, John Negele→Kostas Orginos.
    - Founding EC member John Negele continues to be very active; Winner of 2014 Herman Feshbach Prize.

Scientific Program Committee

Anna Hasenfratz (chair, Colorado), Tom Blum (Connecticut), Will Detmold (MIT), Steve Gottlieb (Indiana), Kostas Orginos (William and Mary), Peter Petretzky (BNL), Ruth Van de Water (Fermilab)

Present today.

Former chairs: Robert Edwards, Frithjof Karsch, Andreas Kronfeld, Claudio Rebbi

The SPC creates a program to accomplish the goals set forth in USQCD's computing proposals.
- It may also advise us on needed evolution of the goals.
- It examines submitted physics proposals in light of the desired program.
- In principle, it could state in the Call For Proposals that proposals in a certain area would be welcome; has not seen the need to do that yet.
- The SPC is programmatic without being top-down.

33 people have served so far as members of the EC and/or the SPC.
The Executive Committee seeks the advice of the SPC on physics priorities when writing new proposals for DoE computing resources.

Chair rotates every two years. Members rotate every four years, at a rate of about two/year.

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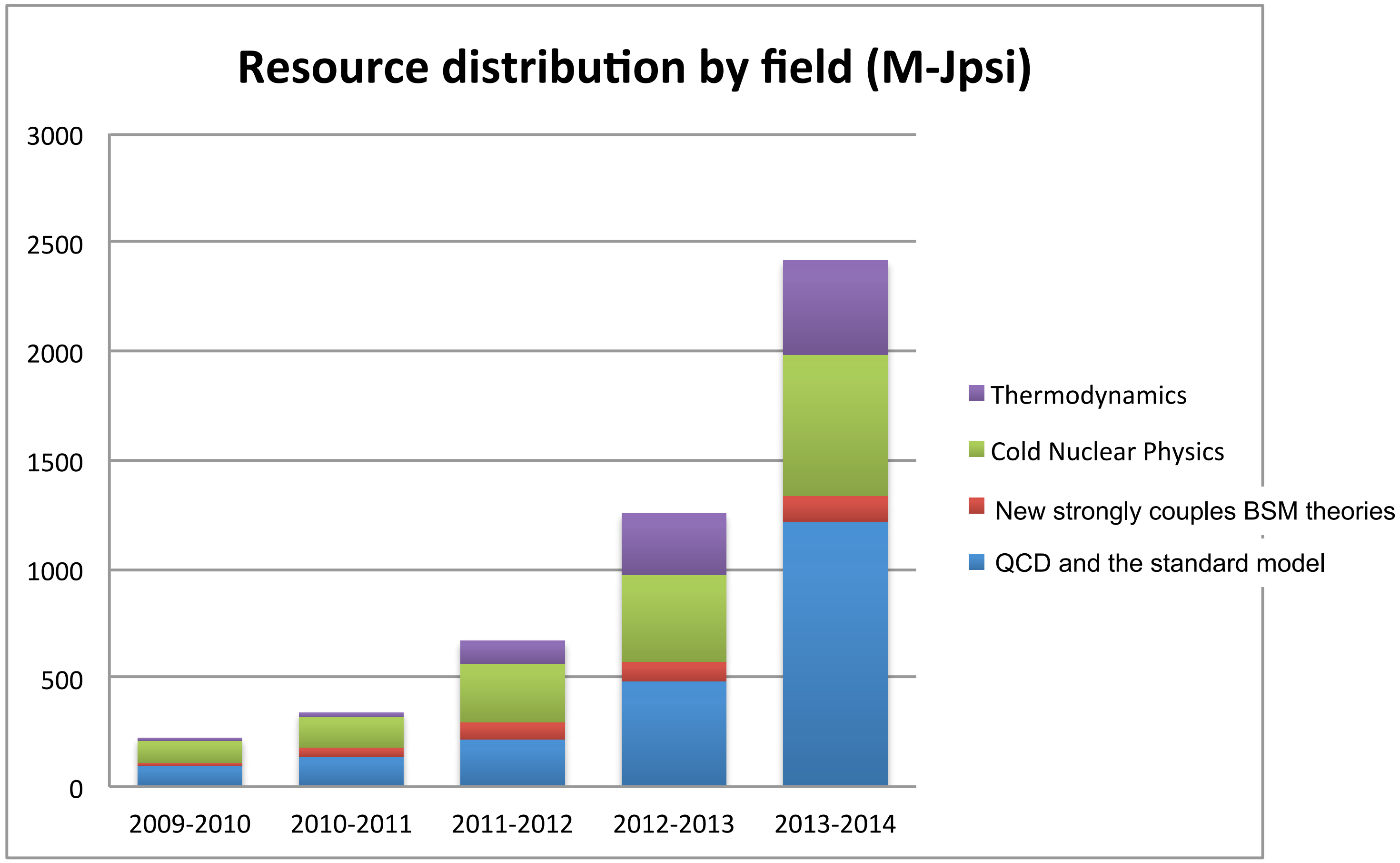
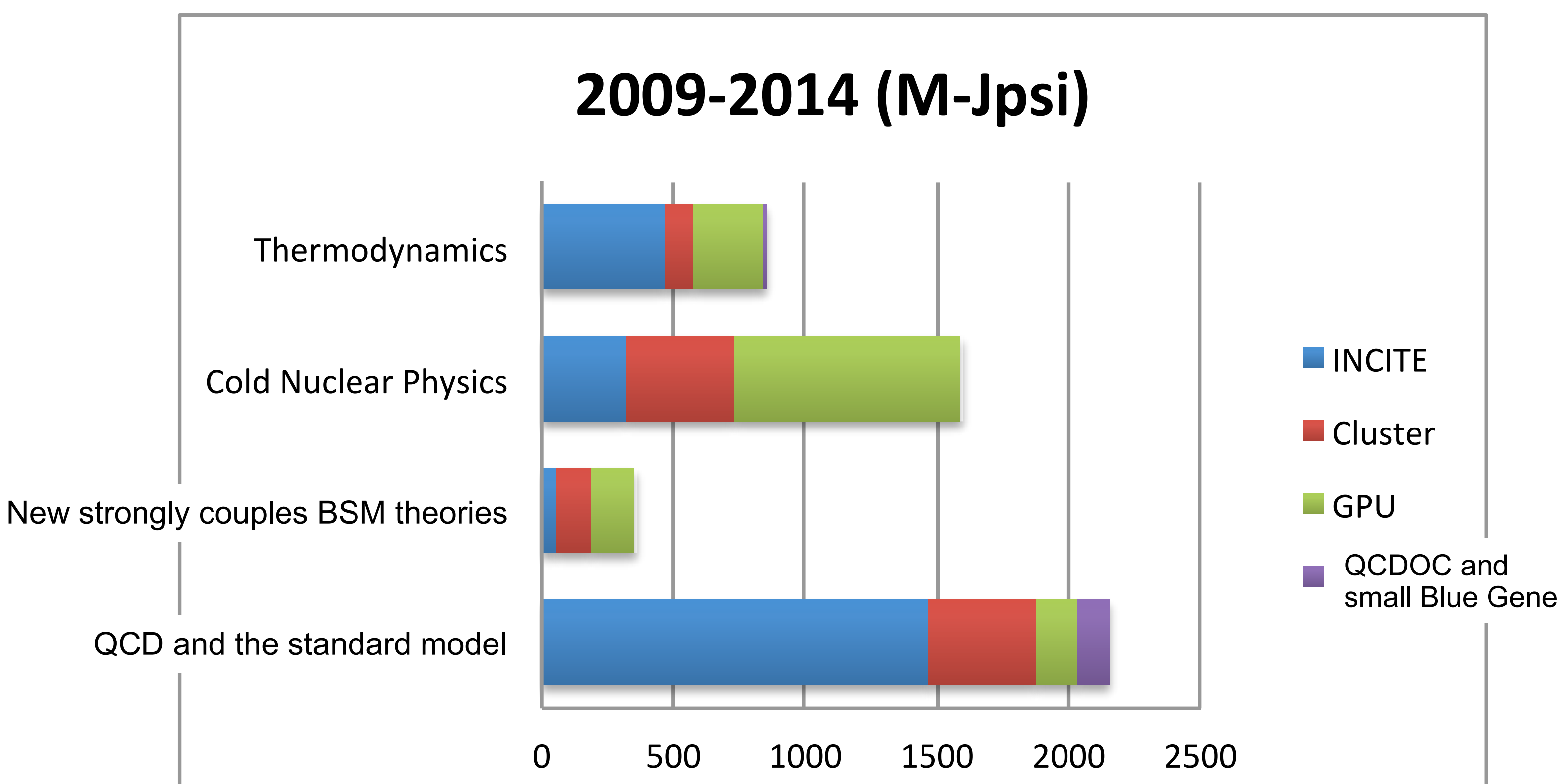
SPC allocations process

- The SPC determines the available resources for the upcoming year.
- After approval from the EC, the SPC issues the Call-for-Proposals.
- The SPC collects and reviews the proposals. Further information is often requested from the proposers.
- After deliberation, the SPC arrives at an allocation through an internal vote.
- Recommendations for allocation are submitted to the EC for approval. The facility managers are also consulted.
- The SPC notifies the PIs and gives a report.

Allocations

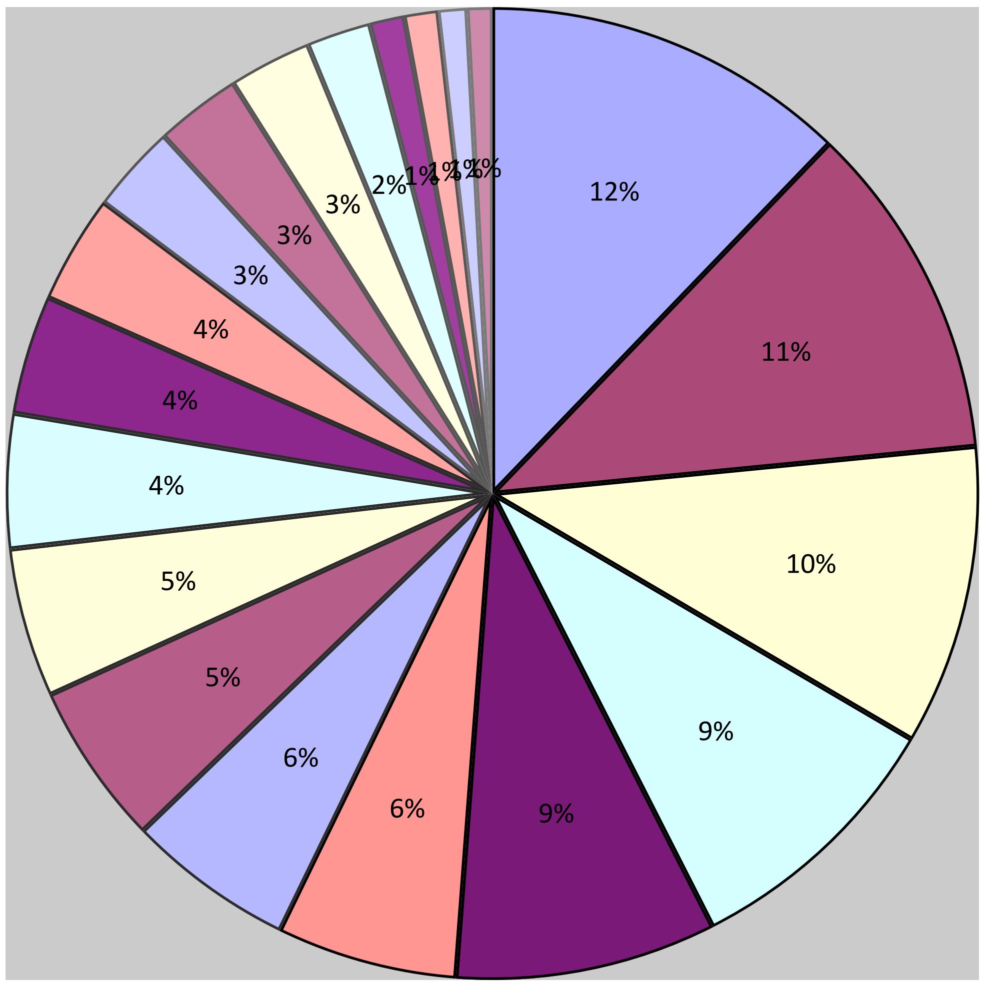




Final allocations for 2015 are not yet available, but the distribution is similar.

Allocations

Type A cluster allocations in 2014 by project.



Projects are judged by:
- relevance to the central goals of USQCD;
- size and competence of project team;
- validity and efficiency of methods proposed.

Less high priority projects are typically not zeroed out, but are given less resources. About half of these allocations went to the five highest priority projects (an HEP project producing a dozen high-priority weak matrix elements, an NP project calculating resonance spectra for Gluex, ...).

(Different from experimental programs, where experiments must be voted either up or down.)

USQCD science goals

2013 USQCD white papers at http://www.usqcd.org/collaboration.html

- The physics goals of USQCD are set out in our proposals and white papers organized by the Executive Committee.
  - 2013 white papers are the most recent statement of our view of our most important goals and opportunities, and our view of our highest impact results; had 23 authors.
  - Continually evolving, in consultation with the SPC.
  - Discussed by USQCD members at All Hands meetings.

Community planning

- Community planning documents are influential in formulating our goals.
  - We participate in creating them, and community needs influence our lattice program.
- We have been active in creating the NSAC long-range plan.
  - See https://www.phy.anl.gov/nsac-lrp/Whitepapers/ , especially EIC, FSNu, HotQCD, QCDHadron, LENP and RHIC-Spin documents for lattice-related material.
- We were active in HEP community planning exercises Snowmass 2013 leading up to the P5 process.
  - See http://www.slac.stanford.edu/econf/C1307292/docs/ComputingFrontier/Lattice-44.pdf .

Science Advisory Board

- In setting and updating our goals we have always relied on informal input from numerous experimenters and phenomenologists.
- Last year, we formalized this process by naming a Science Advisory Board.
  - Brendan Casey (Fermilab, g-2), Daniel Cebra (UC Davis, STAR), Jesse Thaler (MIT), David Kaplan (U. Washington), Curtis Meyer (Carnegie Mellon, GlueX), Alan Schwartz (Cincinnati, Belle), Volker Koch (LBL).
  - Among the most useful advisors on white papers and proposals.
- At the beginning of each year's allocation process, they are asked to
  - Comment and suggest revisions of our general goals,
  - Read and comment on the year's physics proposals and allocations,
    - We are exploring how closely our advisors would like to be involved with the allocations process.

Input from the 2014 and 2015 SABs

- Useful comments on USQCD program,
  - as food for thought. E.g., the lattice HEP program would be stronger if it reflected more faithfully the HEP experimental program of the next few years,
  - or because they reflected a need to improve our message.
- USQCD allocations process
  - "I find the proposals I read mostly pretty well written, with a science justification in the intro, the abstracts are all remarkably of the same format: brief science justification, goals, requested allocation, which is pretty accessible (without being asked to judge whether the project is realistic)...I do not actually imagine that the SAB is going to have much useful feedback for you, but sharing this information might impress the people on the board about what a diverse and active community this is."
- Scientific Program
  - "The g-2, GlueX spectroscopy, proton charge radius, and 3-neutron force computations are of great interest to the community at large, and the first two are given special urgency by specific upcoming experiments. The PDFs, other nucleon form factors, and edm measurements are interesting, but seem to lack the time criticality as far as I can tell."

Detailed comments of SAB members are on the review web site.

2015 USQCD all-hands meeting

- Took place May 1-2, 2015 at Fermilab. ~45 members attended, plus ~6 remote participants. (http://www.usqcd.org/meetings/allHands2015/.)
- Reports from the Executive Committee, the LQCD-ext Project Manager, the SPC, and the hardware site managers.
- In each science domain, reports from
  - representative physics projects,
  - members of the SPC on the relation between the allocated projects and the long-term goals.

- Group discussion on
  - USQCD scientific program on leadership-class resources..

Lattice meets experiment meetings

To increase the interaction between lattice gauge theory and experiment and phenomenology, members of USQCD have organized a series of workshops with experimenters and phenomenologists.

- SLAC, Sept. 16, 2006, Standard Model physics. With BaBar.
- Fermilab, December 10-11, 2007, “Lattice Meets Experiment” in flavor physics.
- Livermore, May 2-3, 2008, “Lattice Gauge Theory for LHC Physics”.
- JLab, Nov. 21-22, 2008, “Revealing the Structure of Hadrons”, Nuclear.
- BNL, June 8-9, 2009, “Critical Point and Onset of Deconfinement”, QCD thermodynamics.
- BU, Nov. 6-7, 2009, “Lattice Gauge Theory for LHC Physics”. BSM.
- Fermilab, April 26-27, 2010, “Lattice Meets Experiment” in flavor physics.
- BU, 8-10 September 2010, “Sixth Workshop on QCD Numerical Analysis, Boston.
- JLab, Feb. 23-25, 2011, “Excited Hadronic States and the Deconfinement Transition”.
- BNL, Oct. 3-5, 2011, "Fluctuations, Correlations and RHIC low energy runs".
- Fermilab, Oct. 14-15, 2011, “Lattice Meets Experiment: Beyond the Standard Model”.
- Boulder, Oct 28, 2012, “Lattice Meets Experiment 2012: Beyond the Standard Model”.
- George Washington University, Aug. 21-23, 2012, “Extreme QCD”.
- BNL, December 5-6, 2013, “Lattice Meets Experiment 2013: Beyond the Standard Model”.
- Fermilab, March 7-8, 2014, “Lattice Meets Experiment, 2014”.
- BNL, Feb. 26-27, 2015, “Theory and Modeling for the Beam Energy Scan”.
- LLNL, April 23 to 25, 2015, “Lattice for Beyond the Standard Model Physics”.
- BNL, June 10, 2015, “RHIC users' meeting: Beam Energy Scan workshop”.

Membership survey and demographic information

- We are starting to collect membership and demographic information in a more organized way.
  - New membership list. Currently, ~ 160 members.
  - Annual demographic survey in the user survey.

We've grown from about 90 people in 2000 to about 160 today.

About 100 sign proposals to the SPC each year.

61 responded to the user survey this year.

2014:

Job Classification	**Count**
Grad Student - University	4
Postdoc - University	11
Postdoc - Laboratory	6
Faculty - University	25
Research Scientist - University	1
Research Scientist - Laboratory	14
Other	0
Answered Question	61
Skipped Question	0

Grad students undercounted.

Junior faculty and staff job creation

	Year	Research institution, HEP	Research institution, NP	Computational scientist	Teaching college	Industry	Foreign
Christoph Lehner	2014	BNL					
Mei-Feng Lin	2014			BNL			
Stefan Meinel ***	2014	Arizona/BNL					
Hiroshi Ohno	2014						Tsukuba
Heng-Tong Ding	2013						CCNU
Andre Walker-Loud **,****	2013		Wm & Mary/JLab				
Jack Laiho	2013	Glasgow→Syracuse					
Will Detmold **	2013		Wm & Mary →MIT				
Ethan Neil ***	2013	Colorado/BNL					
Christopher Thomas	2013						Cambridge
Ruth Van de Water	2012	BNL→Fermilab					
Brian Tiburzi ***	2011		CUNY/BNL				
Andrei Alexandru *	2011		GWU				
Elvira Gamiz	2011						Granada
Mike Clark	2011					NVIDIA	
Ron Babich	2011					NVIDIA	
Christopher Aubin	2010				Fordham		
Swagato Mukherjee	2010		BNL				
Changhoan Kim	2010					IBM	
Enno Scholz	2009						Regensburg
Taku Izubuchi	2008	BNL					
James Osborn	2008			Argonne			
Chris Dawson	2007	Virginia/JLab					
Nilmani Mathur	2007						Tata Institute
Joel Giedt	2007	RPI					
Matthew Wingate	2006						Cambridge
Jozef Dudek **,****	2006		Old Dominion/JLab				
Jimmy Juge	2006				U. of the Pacific		
Peter Petreczky	2006		BNL				
Balint Joo	2006			JLab			
Kieran Holland	2006				U. of the Pacific		
Kostas Orginos **,****	2005		Wm & Mary/JLab				
George Fleming	2005			Yale			
Tom Blum ***	2003	Connecticut/BNL					
Silas Beane *	2003		UNH→U Wash.				
Total		9	9	4	3	3	7

* NSF Early Career Award
** DoE OJI/Early Career

*** RIKEN/BNL bridge positions
**** JLab joint positions

In 2015: Michigan State is creating three new positions in lattice gauge theory.

USQCD total hardware resources

USQCD resources in April, 2015.
Unnormalized core-hours.

	2015 USQCD resources					
			M units	Units	Total M core-hours	Grand total
LQCD Project	**clusters**	DOE/HEP&NP			451	
	GPUs	"	9.5	GPU hrs	~685	
	BNL BGQ	"			71	
Leadership Class	**LCF INCITE**	DOE/ASCR			280	
(capability)						
	Blue Waters	NSF	30	node hrs	480	
	LCF ALCC	DOE/ASCR				
					473	
General purpose	**NERSC**	DOE/ASCR				
					186	
	XSEDE	NSF		SUs		
					32	
						1973

The LQCD Project, INCITE, and Blue Waters were applied for by USQCD as a whole.
The physics collaborations making up USQCD also apply for time at NERSC, NSF XSEDE, ALCC ..., independently of USQCD,
but these come far short of meeting our physics needs.

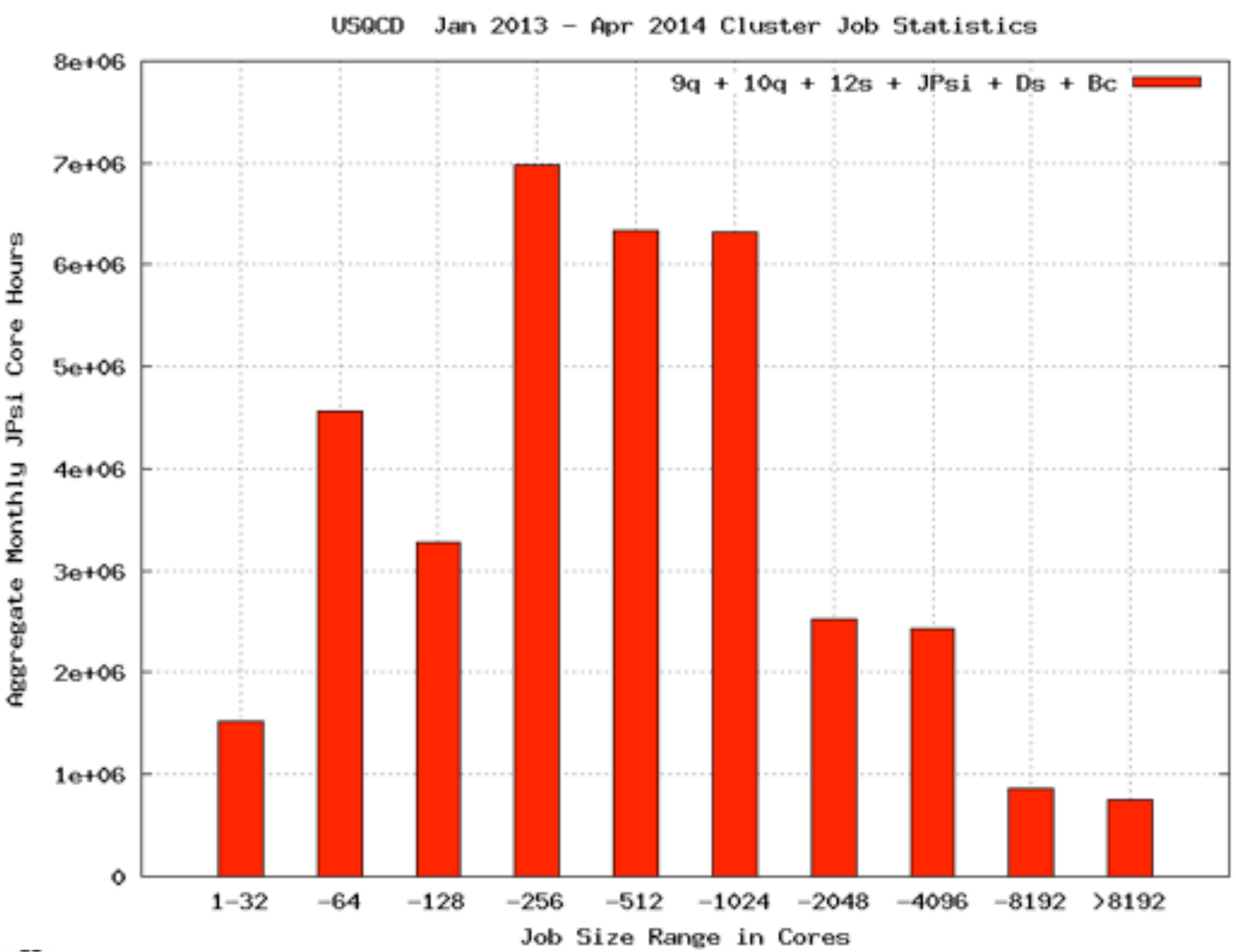
Incite resources

for capability computing.

- The DOE allocates time at its leadership class facilities (LCFs), the Cray/GPU system (Titan) at ORNL and the BlueGene/Q (Mira) at ANL, through its INCITE Program.
    - These are essential for that part of our program requiring high capability computing, such as generation of large gauge configuration ensembles.
- USQCD currently has a three-year grant running from calendar year 2014 though calendar year 2016.
- The USQCD allocation for 2014:
    - 2nd largest INCITE allocation
    - 100 M core-hours on OLCF Titan, 180 M core-hours on ALCF Mira.

Capacity and capability computing

- Leadership class computing is essential for generating large ensembles of gauge configurations. This computing cannot be done any other way.
- We have an even greater need for flops analyzing these configurations.
  - Can often be done very efficiently (cheaply in $/flop) in parallel on much smaller systems.



We have large computing needs at all scales of job-sizes, from one-node jobs to hundred thousand node jobs on a log scale in job-size.

Job size distribution on USQCD 2013/14 conventional clusters.

Capacity and capability computing

- The LCFs are mandated to supply only capability computing needs, jobs that can't be done on any other machines.
  - >128,000 core jobs at ALCF, >3,600 GPU jobs at OLCF.
- Lattice QCD has an even greater need for capacity cycles that LCFs are mandated *not* to supply.
  - The LCFs are well aware that this need exists and are very happy that it is being met because it gives value to the large ensembles we generate there.
- This capacity need can be supplied much more efficiently on dedicated lab clusters than at multipurpose computing facilities.
  - A case study examined by USQCD showed that in one case the USQCD hardware was a factor of three more cost-effective than LCF hardware.
  - Most of our projects are analysis projects requesting more cluster time than INCITE time.

HEP and NP labs are well suited to supply this need.

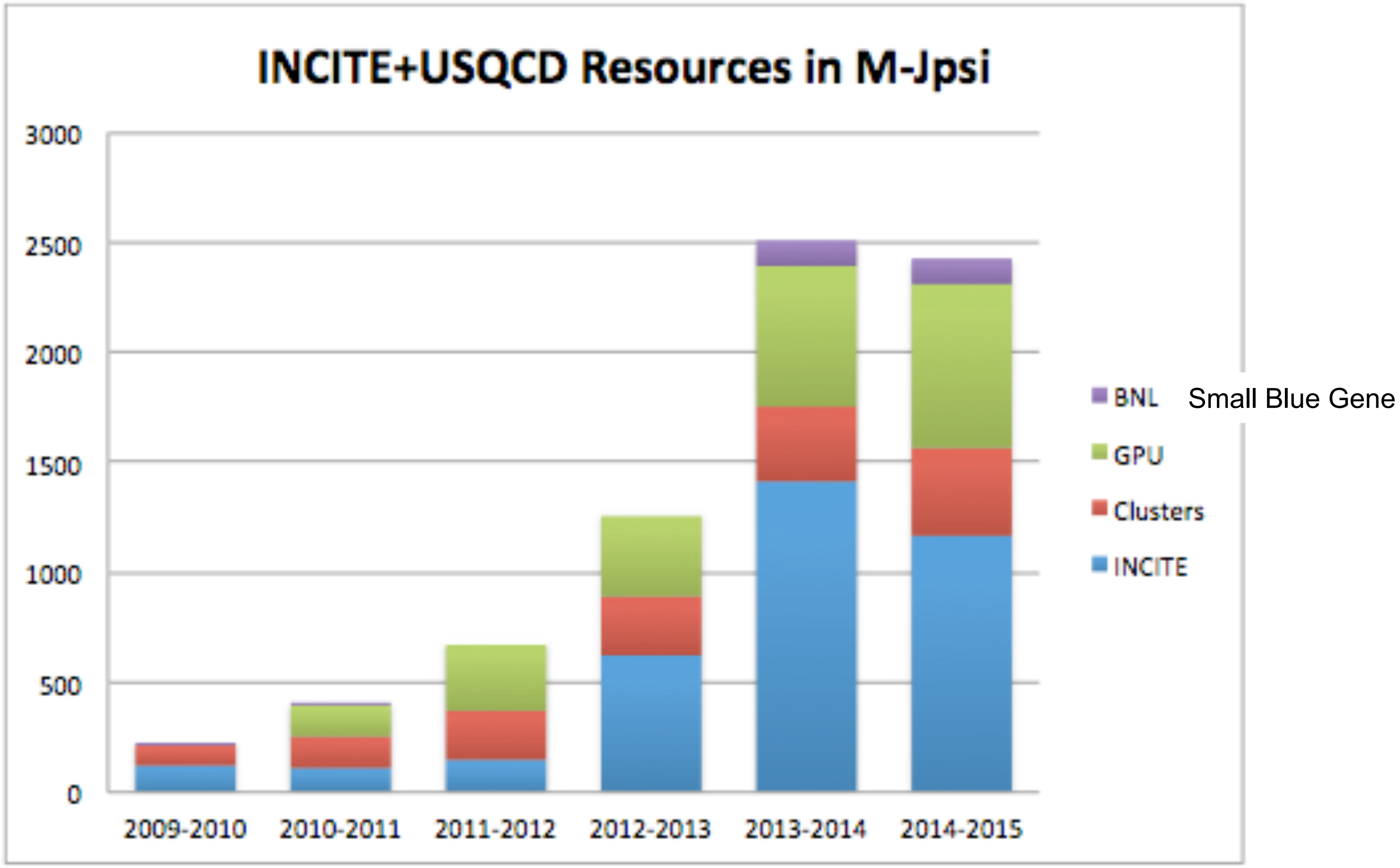
- LQCD clusters leverage lab capabilities.
    - Cluster expertise (reconstruction farms and real time triggers)
    - Storage (networks, file systems, data movement)
    - Lattice clusters exist in an environment of similar but larger experimental clusters for reconstruction and analysis; cycles can be traded back and forth between projects during critical periods, benefiting all concerned.
- LQCD hardware often provides design ideas and prototyping that is useful to other programs at labs and universities.
    - E.g., at Fermilab, for several years Ds-type machines (quad-socket Opterons) have been the standard used for Run 2, FermiGrid, CMS Tier 1;
    - other programs at the labs are now becoming very interested in GPUs and Intel MIC architecture.

GPUs, many-core architectures, ...

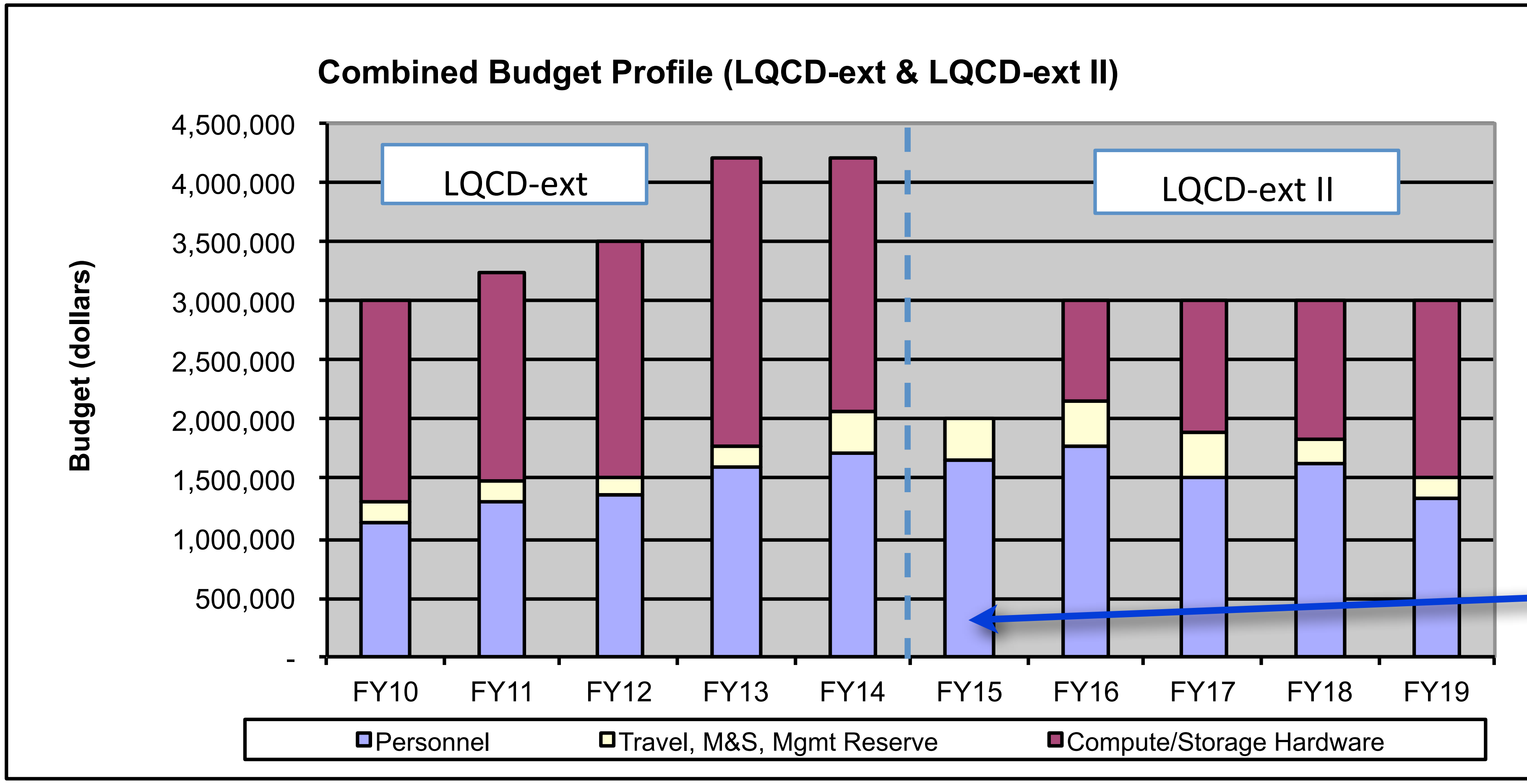
- GPUs have supplied a significant fraction of our capacity computing needs in the last few years.
  - Were a disruptive technology: for the projects that can use them, they provide outstanding price/performance in $, but require significant investments in software and physics brain power.
  - A significant amount of high-level GPU code has now been created.
  - Many of our projects are mature on GPUs, but many are not.
  - Price performance varies much more by project than is true for ordinary clusters.
    - Harder to define a standard candle for price/performance.
  - The speedup we find has been enabled by the terrific work of our software committee.

- Coming chips will continue to become more painful to deal with than the commodity chips of the 2000s.
  - Intel many-core chips are here, a new disruptive technology.
  - Future chips will continue to use more and more cores/chip, more and more layers of memory hierarchy, etc.
- USQCD profits from close relationships with vendors.
  - Former particle physicist Al Gara is now Intel chief exascale architect; was originally part of Norman Christ's lattice QCD computing project at Columbia; was also chief architect of the Blue Gene computers.
  - USQCD member Mike Clark is a full time NVIDIA employee; still a lead USQCD developer and tests future NVIDIA architectures for performance on lattice QCD algorithms.

USQCD hardware resources by year



- Total USQCD hardware resources have risen exponentially following Moore's law for the last few years.
- This will not continue for the next few.
  - This year's trend is flat, and will rise only slowly for the next few.



Under LQCD-ext, we have spent ~ 60% of our funds on hardware, about 40% on operations. Current guidance is for FY15 funding to allow only continued operations - no new hardware purchases.

- Current plans call for reduced and back-loaded funding for LQCD-ext II compared with LQCD-ext, particularly in 2015, a terrible year for HEP.
- The Leadership-class at Argonne and Oak Ridge upgraded their resources by a factor of ~ten in 2013; the next major upgrades planned for ~2017-19.
- USQCD science program will have to adjust for this fact, stretch out science goals, make sure our most important deliverables remain on track.
- Improvements in algorihms and methods will become even more critical.

SciDAC lattice QCD software R&D

The third critical component of our computational infrastructure.

Software Committee: Richard Brower (chair).

Regular Thursday phone conferences for people working on USQCD software.

USQCD has SciDAC-3 grants from HEP+ASCR and NP+ASCR for about $1 M each for creating lattice QCD software infrastructure: community libraries, community codes, optimization and porting to new architectures, implementation of up-to-the-minute algorithm advances...

- The QCD API and community libraries
  - Lower entrance barriers to lattice QCD.
  - Enable postdocs to run major projects without being part of major collaborations.
- Porting and optimizations for new platforms
  - Critical to efficient use of new hardware.
  - Will become even more important over next five years.

Opportunities and Challenges, 2015-2019

- Lattice gauge theory stands today with wider and more important opportunities than ever before.
- But ...
    - In 2005-2014, our support from DoE rose. This will not continue in the coming five years.
    - In the previous ten years, Moore's law progress in chip speeds continued rapidly. This is slowing down.
    - In the previous ten years, commodity hardware performed very well for scientific calculations. Coming chips for scientific computing are becoming increasing complex and hard to program.

Backup slides

Next

- USQCD members: main scientific thrusts
  - The spectroscopy and structure of nucleons and nuclei. Will Detmold.
  - The behavior of QCD in extreme conditions. Frithjof Karsch.
  - Understanding the properties of new strongly interacting gauge theories. Anna Hasenfratz.
  - Testing the Standard Model and the search for new physics in high-precision experiments. Andreas Kronfeld.
- LQCD Project: Project management and computing.

International collaboration

- Lattice QCD is an international field with very strong programs in Germany, Italy, Japan and the United Kingdom, and elsewhere.
- Non-US lattice theorists are welcome to contribute to USQCD projects in collaboration with US theorists.
- Groups within USQCD have formed a number of international collaborations:
  - The USQCD effort using DWF quarks is an international effort between the United States based RBC, the Edinburgh, and Southampton members of the UKQCD Collaboration, and RIKEN.
  - The Fermilab Lattice, HPQCD and MILC Collaborations have worked together in various combinations to study heavy quark physics using improved staggered quarks. HPQCD includes physicists in both USQCD and UKQCD.
  - Members of the BNL Nuclear Physics lattice gauge theory group have a long term collaboration with physicists at the University of Bielefeld, Germany.
  - Members of USQCD working on the hadron spectrum using Clover quarks on anisotropic lattices have close ties with colleagues in Trinity College, Dublin, the Tata Institute, Mumbai, Cambridge U.
  - ...

The computational challenge of lattice QCD

Lattice	Quark			Gauge	ensembles		Analysis propagators, correlators		
spacing *a (fm)*	mass *ml/ms*	Volume (sites)	Configu rations	Core-hours (M)	TB/ ensemble	Files/ ensemble	Core-hours (M)	TB/ ensemble	Files/ ensemble
0.15	1/5	16^3*48	1000	1	0.1	1,000	1	4	155,000
0.15	1/10	24^3*48	1000	2	0.2	1,000	2	12	“
0.12	1/5	24^3*64	1000	3	0.3	1,000	3	16	155,000
	1/10	32^3*64	1000	8	0.6	1,000	8	39	“
	1/27	48^3*64	1000	26	2.0	1,000	26	130	“
0.09	1/5	32^3*96	1000	10	0.9	1,000	10	58	155,000
	1/10	48^3*96	1000	35	3.1	1,000	35	196	“
	1/27	64^3*96	1000	46	7.2	1,000	46	464	“
0.06	1/5	48^3*144	1000	38	4.6	1,000	38	294	155,000
	1/10	64^3*144	1000	128	10.9	1,000	128	696	“
	1/27	96^3*144	1000	218	36.7	1,000	218	2,348	“
0.045	1/5	64^3*192	1000	135	14.5	1,000	135	928	155,000
	1/10	88^3*192	1000	352	37.7	1,000	352	2,412	“
	1/27	128^3*192	1000	1083	116.0	1,000	1,083	7,422	“
0.03	1/5	96^3*288	1000	685	73.4	1,000	685	4,697	155,000
				2,770					

Example gauge ensemble library.

CPU times normalized in JPsi core-hours.

Planned MILC HISQ ensembles of guage configurations. $m_l = 1/27 m_s = m_{phys}$

Operationally, lattice QCD computations consist of

1) Sampling a representative set of gauge configurations with Monte Carlo methods,

   E.g., the Metropolis method, the hybrid Monte Carlo algorithm, ...
   Consists of one long Markov chain. A capability task.

2) Calculating the propagation of quarks through the gauge configurations,

   Solve the Dirac equation on each configuration with relaxation methods, e.g., biconjugate gradient algorithm, etc. A capacity task.

3) Constructing hadron correlation functions from the quark propagators (smaller task).

Two main components of a typical lattice calculation

multi-TB
file sizes

Generate *O*(1,000) gauge configurations on a leadership facility or supercomputer center. Hundreds of millions of core-hours.

Transfer to labs for analysis on clusters. Larger CPU requirements.

Gauge configuration generation:
a single highly optimized program,
very long single tasks,
“moderate” I/O and data storage.

Hadron analysis.
Large, heterogeneous analysis code base,
10,000s of small, highly parallel tasks,
heavy I/O and data storage.

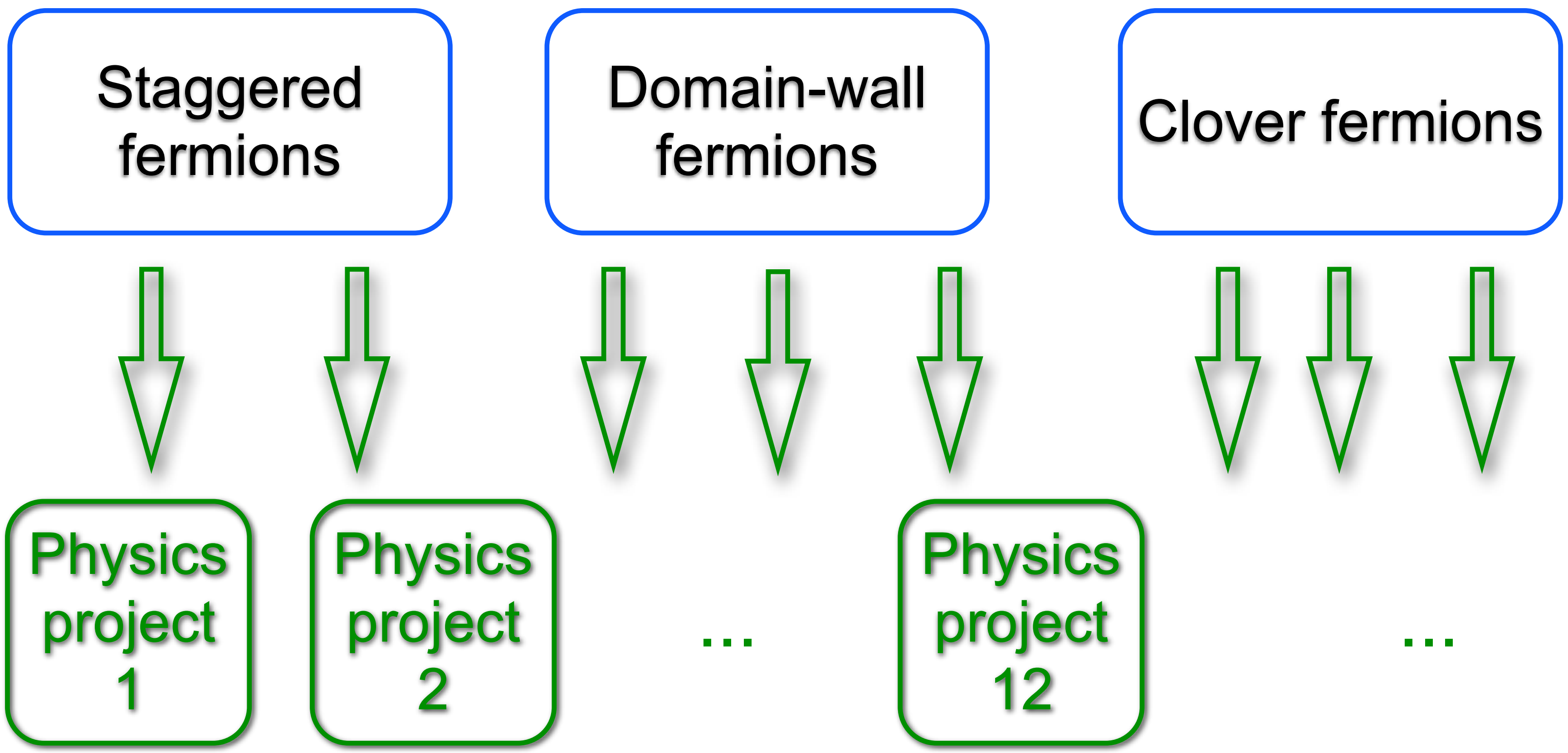
Two comparably sized jobs with quite different hardware requirements.

US lattice gauge theory work flow

Zero-temperature QCD:

Currently three main streams of QCD gauge configurations are being generated by USQCD for different physics goals:

These high-value ensembles are data-rich resources that are shared among all of USQCD.



Shared among a couple of dozen groups, in both HEP and NP.

Physics projects are done on these configurations by smaller groups of 5-15 members within USQCD.

Around 90 of the 163 members of USQCD have submitted jobs to USQCD hardware.

QCD thermodynamics and BSM projects generate their own configurations tailored to specific goals.

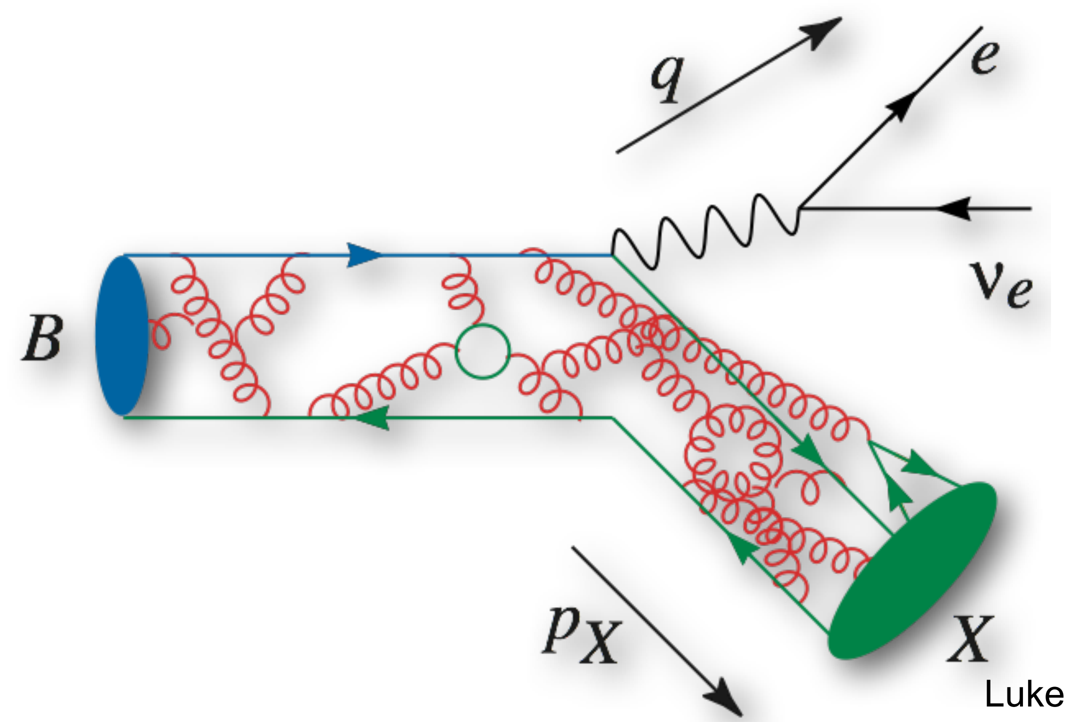
II. Lattice QCD

QCD is the theory of quarks and gluons. Quarks and gluons cannot be directly observed because the forces of QCD are strongly interacting.

Quarks are permanently confined inside hadrons, even though they behave as almost free particles at asymptotically high energies.

"Asymptotic freedom", Gross, Politzer, and Wilczek, Nobel Prize, 2004.

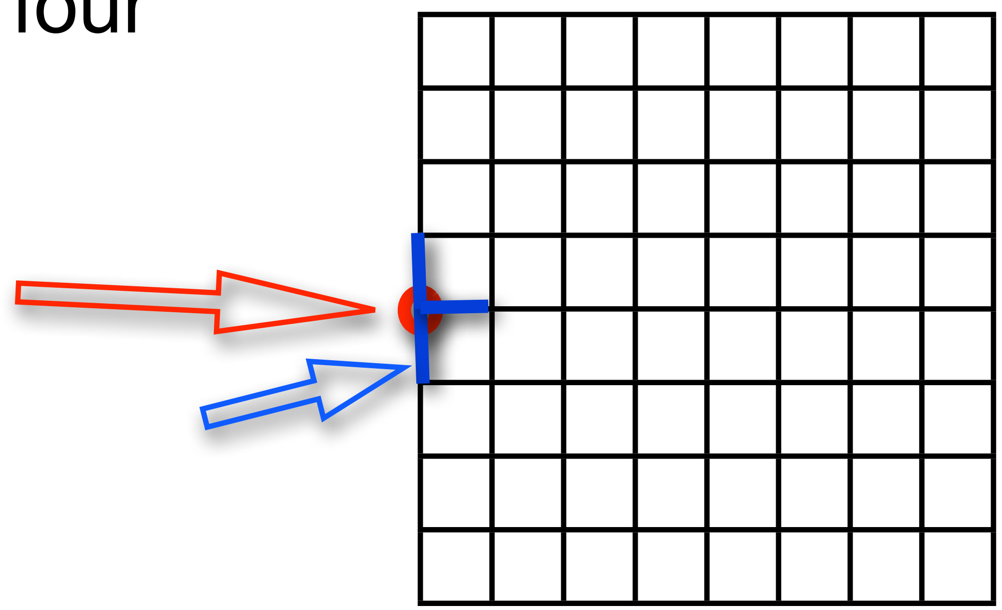
Lattice QCD is used to relate the observed properties of hadrons from the properties of their quark and gluon constituents.



$B \rightarrow \pi l \nu$ semileptonic decay

Lattice quantum field theories

Approximate the path integral of quantum field theory by defining the fields on a four dimensional space-time lattice.



Quarks (ψ) are defined on the sites of the lattice, and gluons (U_μ) on the links.

Monte Carlo methods are used to generate a representative ensemble of gauge fields. Relaxation methods are used to calculate the propagation of quarks through the gauge field.

Continuum quantum field theory is obtained in the zero lattice spacing limit. This limit is computationally very expensive.

The Dirac, or "Dslash", operator

The fundamental operation that consumes the bulk of our cycles is the solution of the Dirac equation on the lattice.

The fundamental component of the Dirac operator is the discrete difference approximation to the first derivative of the quark field on the lattice.

$$\partial_\mu \psi(x) \to \Delta_\mu \psi(x) \approx \frac{1}{2a}(\psi(x+\hat{\mu}a) - \psi(x-\hat{\mu}a)) + \mathcal{O}(a^2)$$

Quarks in QCD come in three colors and four spins.
The color covariant Dslash operator of lattice QCD is

$$D_\mu \gamma_\mu \psi(x) \equiv \frac{1}{2}\left(U_\mu(x)\gamma_\mu \psi(x+\hat{\mu}) - U_\mu^\dagger(x-\hat{\mu})\gamma_\mu \psi(x-\hat{\mu})\right)$$

γ operates on spin four-vector.

U operates on color three-vector of the quark.

The bulk of the flops envisioned in this project are consumed in multiplying complex 3-vectors by 3x3 complex matrices.